

# Isonipecotic acid, N-(cyclohexylcarbonyl)-, tetradecyl ester

**Inchi:** InChI=1S/C27H49NO3/c1-2-3-4-5-6-7-8-9-10-11-12-16-23-31-27(30)25-19-21-28(22-20-26)/1-27  
**InchiKey:** RAVRDPWYQAGKGJ-UHFFFAOYSA-N  
**Formula:** C27H49NO3  
**SMILES:** CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)C2CCCCC2)CC1  
**Mol. weight [g/mol]:** 435.68

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.64		Crippen Method
logp	7.050		Crippen Method
mcvol	388.560	ml/mol	McGowan Method
rinpola	3508.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361037&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpola:** Non-polar retention indices

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